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X-ray diffraction, magnetization, and ^{57}Fe Mössbauer spectroscopic characterization of natural single-crystals of chrysoberyl

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Natural chrysoberyl from Rio das Americanas, Minas Gerais, Brazil, was studied by electron microprobe analysis, X-ray single-crystal diffractometry, magnetization and ^{57}Fe-Mössbauer spectroscopy. The aim of this study is the structural and magnetic characterisation of the sample.

Microprobe measurements of two chrysoberyl crystals were performed with high grid resolution leading to the average chemical composition $Al_{1.96}Fe_{0.03}BeO_4$. The crystals seem to be homogenous.

Single-crystal data were collected and refined on a BRUKER Smart Apex 3-circle diffractometer using the ideal chemical composition, Al_2BeO_4, space group Pnma with four formula units per unit cell and the initial fractional coordinates given by [1]. The results of the refinement show, that the untwinned chrysoberyl has a hexagonal closed packed structure of oxygen ions, slightly distorted with Al^{3+} and Be^{2+} occupying the octahedral and tetrahedral sites of chrysoberyl [2], respectively.

Magnetization data taken down to 3 K reveal paramagnetic moment behavior with S=5/2 as expected for high spin Fe^{3+}. No indications for magnetically ordered impurities were found.

The ^{57}Fe-Mössbauer spectra, collected at different temperatures between 20 K and room temperature, reveal a superposition of several subspectra. Isomer shifts and quadrupole splittings are typical for Fe^{3+} in a comparably weakly distorted six-fold coordination of the M1 and M2 position, the latter with point symmetry m (Al_{II}, 4c-site) in accordance with the EPR measurements of [3]. Remarkable is a strong spectral contribution revealing a magnetic hyperfine splitting, indicative for magnetic order of part of the sample or slow spin relaxation effects. Several scenarios for the origin of this magnetic contribution will be discussed, e.g., defect sites as reported for alexandrite [4], superparamagnetic iron oxide precipitates, or slow paramagnetic spin relaxation of dilute Fe^{3+}.

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